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Fermi resonances in the vibrational spectrum of perfluoroethane

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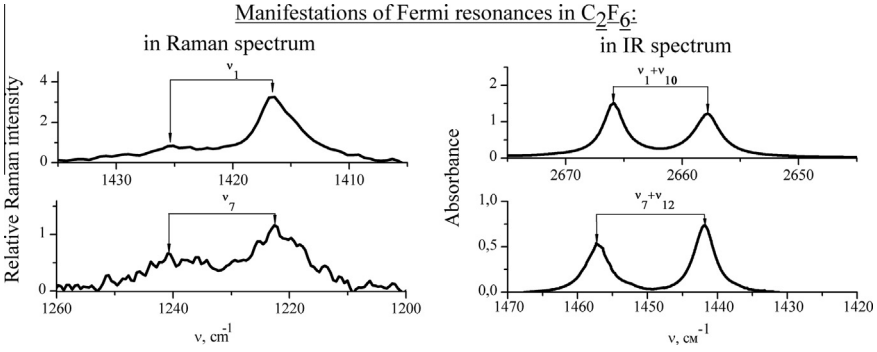
HIGHLIGHTS

- The Raman spectrum of liquid C_2F_6 is presented.
- Data on six fundamental Raman bands of C_2F_6 are obtained.
- Fermi resonances of states $\nu_7 \sim (2\nu_8) \sim (\nu_6 + \nu_{11})$ and $\nu_1 \sim (2\nu_6)$ are detected.

GRAPHICAL ABSTRACT



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ABSTRACT

In this paper the Raman spectrum of liquid C_2F_6 in the spectral region 250–1500 cm^{-1} is presented. Data on six fundamental Raman bands of C_2F_6 are obtained. Doublets are observed in the spectral regions of the ν_1 (A_{1g}) (1416.3 cm^{-1}, 1425.0 cm^{-1}) and ν_7 (E_g) (1221.9 cm^{-1}, 1239.7 cm^{-1}) fundamental bands. The structure of these bands is explained in terms of the Fermi resonances of $\nu_7 \sim (2\nu_8) \sim (\nu_6 + \nu_{11})$ (E_g) and $\nu_1 \sim (2\nu_6)$ (A_{1g}) states. The values of the cubic potential energy constant $K_{166} = 7.7\ (2)\ cm^{-1}$ and the effective matrix element of a threefold interaction $W_{eff} = 8.5\ (5)\ cm^{-1}$ were derived from the simultaneous processing of the doublet parameters in the Raman spectrum of liquid C_2F_6 and in the IR spectrum of C_2F_6 in liquid N_2.

Introduction

Perfluoroethane C_2F_6 is a greenhouse gas emitted into the atmosphere by semiconductor and aluminum industries [1,2]. In this connection optical properties of this molecule attract considerable interest. At present, the Raman spectrum of this molecule is not studied thoroughly. All modern researchers interested in the frequencies of Raman bands of the perfluoroethane molecule (C_2F_6) in the regions of fundamental transitions (for example, in order to estimate the results of ab initio calculation, for example [3,4]) refer to papers [5–7]. This data were obtained in the 1950–1970s.

Interpretation of Raman spectrum of gaseous C_2F_6 in the fundamental spectral region is presented in [6]. The Raman spectrum of liquid C_2F_6 is studied in [5,7]. It is necessary to note that the main purpose of [7] was to study the vibrational spectrum of an α-crystalline phase of perfluoroethane. In addition, the authors of [7] also reported the band frequencies of liquid C_2F_6 but they did not present any spectra of the liquid and data on band intensities.

On the whole, the results of [5–7] are in satisfactory agreement with one another and until recently did not cause doubts. Note that manifestations of intramolecular resonances have not been

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observed in [5–7]. However, the presence of Fermi resonances of states $\nu_1 \sim 2\nu_6$ (A_{1g}) and $\nu_7 \sim 2\nu_8 \sim \nu_6 + \nu_{11}$ (E_g) was recently predicted in paper [8]. According to [8], doublets and more complicated structures are observed in the IR spectrum of solution of C_2F_6 in Xe (T = 163 K) in the spectral regions corresponding to vibrations combined with ν_1 and ν_7, which can only be interpreted with the resonance interactions taken into account. Therefore one can expect Fermi resonance multiplets $\nu_1 \sim 2\nu_6$ (A_{1g}) and $\nu_7 \sim 2\nu_8 \sim \nu_6 + \nu_{11}$ (E_g) to appear in the Raman spectrum of C_2F_6 molecule.

The goals of this work are to measure the Raman frequencies in the spectrum of liquid C_2F_6 more accurately, to determine their relative intensities, and to specify resonance characteristics of higher vibrational states using the IR spectrum of C_2F_6 in liquid N_2 and compare them with the spectrum of C_2F_6 in liquid Xe [8].

Experimental

The Raman spectrum of liquid C_2F_6 was studied on a Nicolet 6700 spectrometer with a NXR FT-Raman Module. A ND: VO4 laser with a working frequency ν = 9398 cm^{-1} and a peak power of 2.5 W was used as a light source. The spectroscopic resolution was 1 cm^{-1}. The functional scheme of the cryostat is shown in Fig. 1.

In the standard observation scheme a laser beam from the source (1) goes through the entrance aperture (3) to the parabolic mirror (4) and strikes a sample (2). The sample (2) should be placed in the focus of the parabolic mirror (the focal length f = 2 cm). It is very difficult to create a cryostat with linear sizes allowing to place the sample into the mirror focus, so we used a light guide for transferring the focus from the sample cell (12) to the sample place (2).

The cell body (6) is made of brass, which ensures even distribution of temperature all over the cell. The sample temperature is controlled both by nitrogen entering the nitrogen chamber (7) and a heating spiral (8). The temperature is measured by a thermocouple (9). The temperature stability of the experiment reached 2 K.

A clamping flange (10), as well as an indium seal (11) make the fastening of the light guide to the cell body leakproof. One end of the light guide is placed inside the working volume (12), the other in the focus of the parabolic mirror (2).

The light guide diameter is compatible with the size of the entrance aperture (3) in the parabolic mirror (4) and equals 5 mm.

The light guide is 5 cm long and it serves two purposes: to transfer the focus (2) into the working volume (12) and to choose a temperature gradient. C_2F_6 enters the working volume (12) in a gas phase and next condenses due to temperature reduction.

A spherical mirror for collecting scattered light in the working volume is fastened to the flange (13). The mirror has a curvature radius equal to 1 cm. The working volume is a space in the cryostat filled with investigated substance where scattering occurs.

The experiment was done at a temperature of 178 (5) K. The observed spectrum is presented in Fig. 2. Intensities of the bands observed in the spectrum were determined relative to the strongest ν_2 band, its intensity assigned taken to be 100 relative units.

IR absorption spectra of C_2F_6 in liquid N_2 were recorded in the same way as described in paper [9].

It is important to note that when interpreting the Raman and absorption bands we used the numbering of normal modes according to [9].

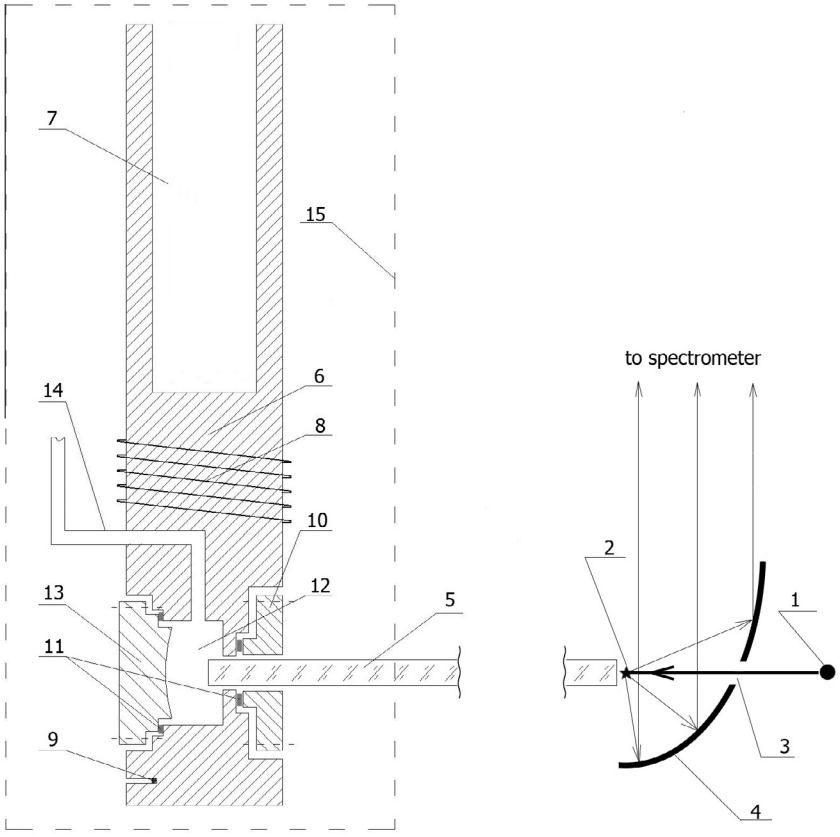

Fig. 1. Functional scheme of cryostat. (1) – Laser beam, (2) – sample place, (3) – entrance aperture, (4) – parabolic mirror, (5) – light guide, (6) – cell body, (7) – nitrogen chamber, (8) – heating spiral, (9) – thermocouple, (10) – clamping flange, (11) – indium seal, (12) – sample cell, (13) – flange with a spherical mirror, (14) – inlet for the substance, and (15) – heat-insulating cover.

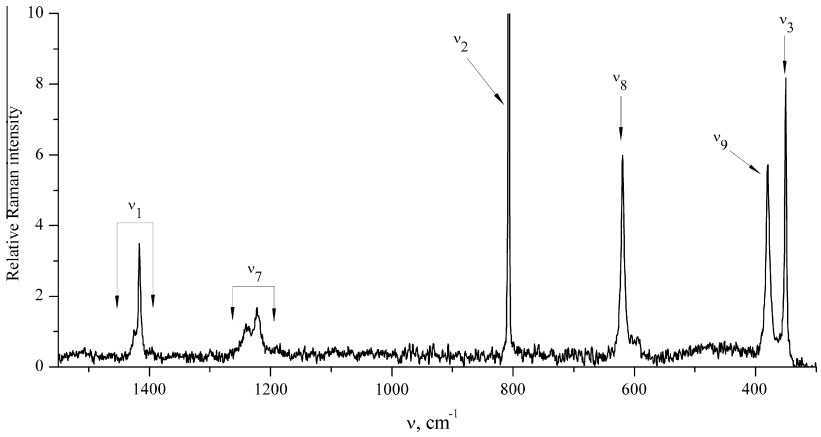

Fig. 2. Fundamental region of the Raman spectrum of liquid C_2F_6 at $T = 178$ (2) K.

Results and discussion

The Raman spectrum parameters of liquid C_2F_6 (frequencies, full widths at half maximum (FWHM), and relative intensities) are presented in Table 1. The analogous data from [5–7] are also presented for comparison. The fundamental frequencies of modes ν_2, ν_3, ν_8 and ν_9 are in good agreement with the data of [5–7]. In [5] the band at 655 cm^{-1} was interpreted as $2\nu_{12}$, but in other studies this band was not observed (we have not observed it either).

Table 1 shows that the intensities of the doublet components in the ν_1 spectral region are of the same order of magnitude. Such correlation of intensities of bands of the first and second orders is possible in the case of a Fermi resonance interaction of these states. The Fermi resonance occurs in the case of an identical symmetry of the interacting states; therefore, we consider the doublet in question as a manifestation of Fermi resonance of states ν_1 (A_{1g}) and $2\nu_6$ (A_{1g}) in the Raman spectrum of C_2F_6. In this connection we believe the interpretation of this doublet as ν_1 (A_{1g}) and $\nu_2 + \nu_8$ (E_g) bands in [7] to be incorrect. A doublet with maxima at 1221.9 cm^{-1} and 1239.7 cm^{-1} is observed in the spectral region of ν_7 band, the intensities of the doublet components being of the same order (Table 1). The authors of [7] also observed two bands at frequencies 1223 cm^{-1} and 1242 cm^{-1} and interpreted them as ν_7 (E_g) and $2\nu_8$ (E_g), respectively. At the same time the frequency of $\nu_6 + \nu_{11}$ (E_g) is close to that of ν_7 [9]. To illustrate this point, let us consider the sum of appropriate fundamental frequencies: $(\nu_6 + \nu_{11}) = 714 + 522.5 = 1236.5$ cm^{-1}; $2\nu_8 = 2(\nu_8) = 2{\cdot}619.5 = 1239$ cm^{-1}; $\nu_7 = 1237$ cm^{-1} (the frequencies are taken from [9]). Consequently, it is necessary to consider resonance interaction of the three (E_g) states ν_7, $(\nu_6 + \nu_{11})$ and $2\nu_8$ through cubic constants of potential energy $K_{67,11}$ and K_{788}. In the present study we determine the cubic constants K_{ijk} of intramolecular potential function $V(q)$ represented by a power series expansion in products of dimensionless normal molecular coordinates q [10]: $V(q) = (1/2)\sum_i \omega_i q_i^2 + \sum_{ijk} K_{ijk} q_i q_j q_k + \cdots$.

The results of measurements of frequencies and intensities of Fermi multiplets in the IR spectra of C_2F_6 in liquid N_2 are presented in Table 2. The table demonstrates manifestation of the same resonances of all observed states combined with ν_1 and ν_7 vibrations.

Let us consider the Fermi doublets in the ν_1 and ν_7 spectral regions in more detail (Fig. 3a and b). In both spectral regions one can observe two bands with close intensities, the components of each doublet being described by Lorentz contours, which makes it possible to determine the quantitative characteristics of Fermi resonance.

Once the experimental values of splitting (χ) and relative intensities of the doublet (R) are obtained, one can define resonance detuning $\Delta = \chi(1 - R)/(1 + R)$ and interaction matrix elements of states $W = \sqrt{\chi^2 - \Delta^2}/2$.

Thus, the $\nu_1 \sim 2\nu_6$ (A_{1g}) resonance appears in all states combined with ν_1 in IR absorption spectra (Fig. 4).

Table 1
Experimental frequencies ν_i, (cm^{-1}), FWHM (cm^{-1}) and relative intensities of some fundamental and combined Raman bands of liquid C_2F_6, $T = 178$ K (this work) as compared with the literature data.

Assignment	ν_i, cm^{-1}	FWHM, cm^{-1}	Raman intensity, relative units	ν, cm^{-1} [5]	ν, cm^{-1} [6]	ν, cm^{-1} [7]
ν_3, A_{1g}	350.4	3.2	20.2	349	348	351
ν_9, E_g	380.2	7.3	30.8	380	372	381
ν_8, E_g	619.4	5.7	29.0	620	619	620
$2\ \nu_{12}$, A_{1g}, E_g	–	–	–	655	–	–
ν_2, A_{1g}	807.5	1.2	100	809	807.4	807
ν_7 / $2\nu_8$ / $\nu_6 + \nu_{11}$, E_g	1221.9 1239.7	14 11	13.9 9.0	1237	1250	1223 1242(1)
ν_1 / $2\nu_6$, A_{1g}	1416.3 1425.0	4.3 7.2	17.6 6.2	1420	1417	1417 1426(2)

Notes: 1 – the authors of [7] interpreted this band as ($2\nu_8$, E_g), 2 – the authors of [7] interpreted this band as ($\nu_2 + \nu_8$, E_g).

Table 2
Experimental frequencies ν_i (cm^{-1}), FWHM (cm^{-1}), and intensities of combination absorption bands (A) of C_2F_6 in liquid nitrogen, $T = 77$ K.

Assignment	ν_i, cm^{-1}	FWHM, cm^{-1}	A, km/mol
$\nu_7 + \nu_{12}$ / $\nu_6 + \nu_{11} + \nu_{12}$ / $2\nu_8 + \nu_{12}$	1442.0 1457.4	3.6 3.6	1.3 0.8
$\nu_1 + \nu_{12}$ / $2\nu_6 + \nu_{12}$	1632.9 1642.2	2.3 2.5	0.8 0.2
$\nu_1 + \nu_6$ / $3\nu_6$	2126.3 2139.7	1.5 1.5	0.065 0.045
$\nu_7 + \nu_{10}$ / $2\nu_8 + \nu_{10}$ / $\nu_6 + \nu_{10} + \nu_{11}$ A_{2u}	2455.3 2477.7	4.5 5.1	0.6 0.3
$\nu_7 + \nu_{10}$ / $2\nu_8 + \nu_{10}$ / $\nu_6 + \nu_{10} + \nu_{11}$ E_u	2465.5 2482.2	5.0 6.0	1.9 3.1
$\nu_1 + \nu_{10}$ / $2\nu_6 + \nu_{10}$	2657.8 2665.7	2.9 2.5	1.65 1.45

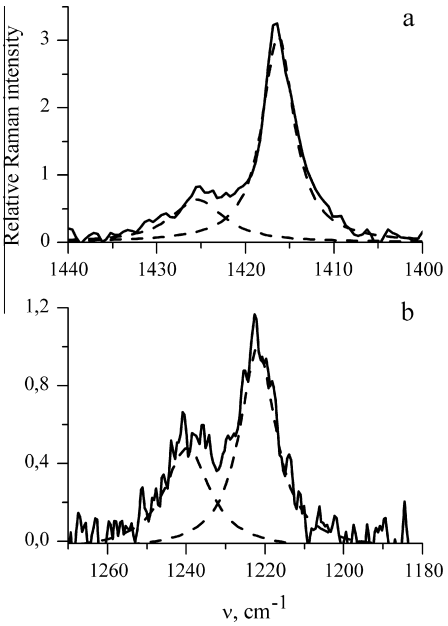

Fig. 3. Raman spectrum of liquid C_2F_6 (T = 178 K) in spectral regions of ν_1 band (a) and ν_7 band (b). The dashed curve shows the Lorentz contours describing the band shapes.

Table 3 presents the results of processing of the experimental data obtained from the Raman spectrum of liquid C_2F_6 and IR spectra C_2F_6 in liquid N_2 and in liquid Xe [8] in the spectral region of the ν_1 band and those containing ν_1.

It is evident that the values of χ and R considerably depend on the experimental conditions. At the same time the values of W coincide to within the experimental error, except for the $\nu_1 + \nu_6$ spectral region. The value of W varies with the quantum numbers of interacting states: $W(\nu_1 \sim 2\nu_6) = K_{166}/2, W(\nu_1 + \nu_6 \sim 3\nu_6) = \sqrt{3}K_{166}/2$. Combined processing of data on all the doublets gives the value of the cubic constant K_{166} = 7.7 (2) cm^{-1}.

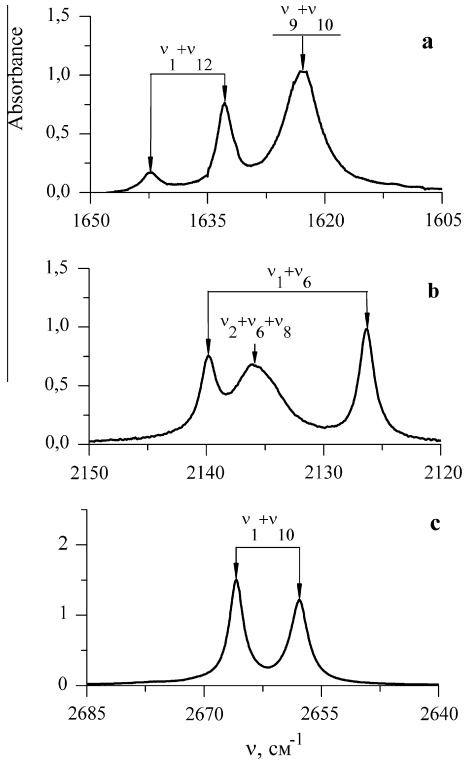

Fig. 4. Absorption spectra of C_2F_6 solution in liquid N_2 (T = 77 K, l = 2.5 cm, $C = 1.2 * 10^{-5}$ mol/cm^3) in $\nu_1 + \nu_{12} \sim 2\nu_6 + \nu_{12}$ (a), $\nu_1 + \nu_6 \sim 3\nu_6$ (b) and $\nu_1 + \nu_{10} \sim 2\nu_6 + \nu_{10}$ (c) spectral regions.

Table 3
Experimental frequencies (ν_i) and parameters of Fermi resonance $\nu_1 \sim 2\nu_6$ obtained from Raman spectra of liquid C_2F_6 (T = 178 K) and solutions of C_2F_6 in liquid Xe (163 K) [8] and N_2 (T = 77 K): splitting (χ), relative intensities of doublet (R), interaction matrix elements of states (W) and resonance detuning (Δ).

Resonance	System, activity	ν_i, cm^{-1}	χ, cm^{-1}	R	W, cm^{-1}	Δ, cm^{-1}
ν_1 $2\nu_6$	Liq. C_2F_6, Raman	1417.5 1424.8	8.7 (2)	0.35	3.8 (1)	4.2 (5)
$\nu_1 + \nu_{10}$ $2\nu_6 + \nu_{10}$	C_2F_6/Liq. Xe [8], IR	2651.0 2659.8	8.8 (2)	0.60	4.2 (1)	−2.2 (4)
	C_2F_6/Liq. N_2 IR	2657.8 2665.7	7.9 (2)	0.90	3.9 (1)	0.4 (4)
$\nu_1 + \nu_6$ $3\nu_6$	C_2F_6/Liq. Xe [8] IR	2123.0 2136.6	13.6 (2)	0.57	6.4 (1)	3.8 (7)
	C_2F_6/Liq. N_2 IR	2126.3 2139.7	13.4 (2)	0.67	6.5 (1)	3.7 (5)
$\nu_1 + \nu_{12}$ $2\nu_6 + \nu_{12}$	C_2F_6/Liq. N_2 IR	1632.9 1642.2	9.3 (2)	0.25	3.7 (2)	5.6 (5)

In the ν_7 spectral region interaction of three vibrational states (a threefold resonance) should be taken into account. The secular equation can be presented as follows:

$$\begin{vmatrix} E_1^0 - \lambda & W_1 & W_2 \\ W_1 & E_2^0 - \lambda & 0 \\ W_2 & 0 & E_3^0 - \lambda \end{vmatrix} = 0,$$

where E_i^0 represents the energy values unperturbed by resonance; $W_1 = K_{788}/\sqrt{2}$; $W_2 = K_{67,11}/2\sqrt{2}$. The matrix element of interactions of vibrational states $2\nu_8$ with $\nu_6 + \nu_{11}$ is too small to be taken into consideration.

Such threefold resonances were discussed in more detail in [11]. The paper [11] shows that a threefold resonance appears in the form of a doublet in the case where the interaction matrix elements are larger than the splitting of unperturbed levels E_2 ($\nu_6 + \nu_{11}$) and E_3 ($2\nu_8$).

In such case it is only possible to obtain a value of an «effective» matrix element of interaction $W_{eff.} = \sqrt{W_1^2 + W_2^2}$ from experimental data, the average of the values makes W_{eff} = 8.5 (5) cm^{-1}. We should also note that the bands corresponding to vibrations combined with ν_7 have a doublet structure both in the Raman and IR spectra (Figs. 3a and 5).

Table 4 presents the results of experimental data processing obtained from the Raman spectrum of liquid C_2F_6 and IR spectra C_2F_6 in liquid N_2 and in liquid Xe [8] in ν_7 spectral region and those containing ν_7.

To illustrate the correctness of these interpretations, the optimized geometry and vibrational frequencies were calculated in the ab initio Møller–Plesset second-order (MP2) frozen core approximation [12] with the Pople-type 6-311++G(df,pd) basis set by the Gaussian 09 package [13]. The anharmonic frequencies and the cubic anharmonicity constants were calculated using the option "anharmonic".

The ab initio calculation of the molecule C_2F_6 gives a value of the cubic constant K_{166} = 6.6 cm^{-1}, the corresponding experimental value is K_{166} = 7.7 (2) cm^{-1}.

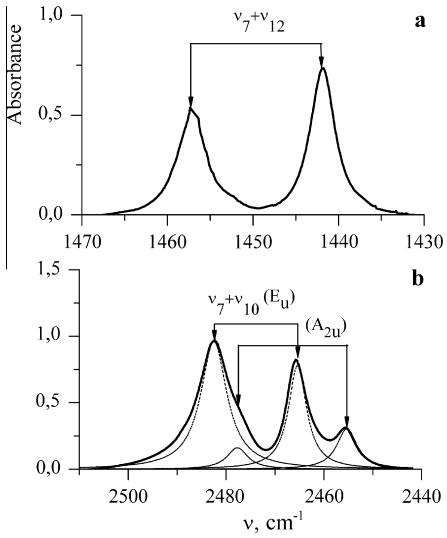

Fig. 5. Absorption spectra of C_2F_6 solution in liquid N_2 (T = 77 K, l = 2.5 cm, $C = 1.2 * 10^{-5}$ mol/cm^3) in the $\nu_7 + \nu_{12} \sim 2\nu_8 + \nu_{12} \sim \nu_6 + \nu_{11} + \nu_{12}$ (a), $\nu_7 + \nu_{10} \sim 2\nu_8 + \nu_{10} \sim \nu_6 + \nu_{10} + \nu_{11}$ (b) spectral regions. The dotted lines represent Lorentz contours describing the multiplet components. In the region of $\nu_7 + \nu_{10}$ vibration (Fig. 5b) there are two doublets (one having symmetry A_{2u} and the other – E_u).

Table 4
Experimental frequencies (ν_i) and parameters of Fermi resonance $\nu_7 \sim 2\nu_8 \sim \nu_6 + \nu_{11}$ obtained from Raman spectra of liquid C_2F_6 (T = 178 K) and solutions of C_2F_6 in liquid Xe (163 K) [8] and N_2 (T = 77 K): splitting (χ), relative intensities of doublet (R), effective interaction matrix elements of states (W_{eff}) and resonance detuning (Δ).

Resonance	System, activity	ν_i, cm^{-1}	χ, cm^{-1}	R	Δ, cm^{-1}	W_{eff}, cm^{-1}
ν_7 $\nu_6 + \nu_{11}$ $2\nu_8$	Liq. C_2F_6, Raman	1221.9 1239.7	17.8	0.6 (1)	9 (1)	8.6 (4)
$\nu_7 + \nu_{12}$ $\nu_6 + \nu_{11} + \nu_{12}$ $2\nu_8 + \nu_{12}$	C_2F_6/Liq. Xe [8], IR C_2F_6/Liq. N_2 IR	1440.0 1456.0 1442.0 1457.4	16.0 15.4 	0.75 (5) 0.8 (1)	2.3 (5) 2.2 (9)	7.9 (1) 7.6 (1)
$\nu_7 + \nu_{10}$ $\nu_6 + \nu_{10} + \nu_{11}$, A_{2u} $2\nu_8 + \nu_{10}$	C_2F_6/Liq. N_2 IR	2455.3 2477.7	22.4 	0.50 (5)	8 (1)	10.6 (2)
$\nu_7 + \nu_{10}$ $\nu_6 + \nu_{10} + \nu_{11}$, E_u $2\nu_8 + \nu_{10}$	C_2F_6/Liq. Xe [8], IR C_2F_6/Liq. N_2 IR	2458.9 2475.4 2465.5 2482.2	16.5 16.7 	0.60 (5) 0.60 (5)	4.1 (7) 4.2 (7)	8.0 (1) 8.1 (1)

The ab initio calculation gives the values of cubic constants $K_{67,11} = -18.2$ cm^{-1} and $K_{788} = 5.4$ cm^{-1}, which enables us to determine the corresponding matrix elements of interaction $\nu_7 \sim (2\nu_8) \sim (\nu_6 + \nu_{11})$ states as $W_1 = K_{788}/\sqrt{2} = 3.8$ cm^{-1}, $W_2 = K_{67,11}/2\sqrt{2} = 6.4$ cm^{-1}. Thus, according to the calculation, the value of the "effective" matrix element of interaction is $W_{eff} = 7.4$ cm^{-1}, the corresponding experimental value is $W_{eff} = 8.5\ (5)$ cm^{-1}. It is evident that the experimental and calculated values of "effective" matrix elements for a threefold resonance $\nu_7 \sim (2\nu_8) \sim (\nu_6 + \nu_{11})$ are in good accordance with each other. We note that the value of W_{eff} is close to W_2 and the shape of the spectrum is determined, above all, by the resonance interaction of ν_7 and $(\nu_6 + \nu_{11})$ states.

Conclusions

In this paper we described the doublets in the Raman spectrum of liquid C_2F_6 in the spectral regions of ν_1 and ν_7 bands. The corresponding resonances of high vibrational states are observed in absorption spectra of C_2F_6 in liquid N_2. The calculated cubic anharmonicity parameters determine the form of molecular vibrational spectra, both in Raman and IR regions. For a proper interpretation of vibrational spectra it is necessary to consider interactions of all the three states $\nu_7 \sim (2\nu_8) \sim (\nu_6 + \nu_{11})$ (all of them have the E_g symmetry).

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